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Gram-Charlier development of the atomic displacement factors into mineral structures: The case of samsonite, $Ag_4MnSb_2S_6$

Luca Bindi[1,*] and Michel Evain[2]

[1]Dipartimento di Scienze della Terra, Università degli Studi di Firenze, Via La Pira, 4-I-50121 Firenze, Italy
[2]Laboratoire de Chimie des Solides, IMN, UMR C6502 CNRS, Université de Nantes, 2 rue de la Houssinière, BP32229, 44322 Nantes CEDEX 3, France

Abstract

During structure solution of Ag-, Cu-bearing minerals it is quite common to observe disorder. Ag^+ and Cu^+, indeed, can occur in different, but overlapping sites. The typical way to deal with these kind of minerals in structure determination is to use a split-atom model. This approach, however, has several disadvantages and may give rise to ambiguities. A solution to the problem can be the use of higher order tensor elements in the expression of the structure factors (the "non-harmonic approach"). This alternative approach gives, in cases of highly overlapping electron densities, an equivalent description of the split-atom model.

The non-harmonic approach based upon a Gram-Charlier development of the atomic displacement factors can be useful in mineral sciences for the determination of still unknown structures. In addition, such an approach can be used to refine known structures with suspiciously high *R* values and/or high isotropic displacement parameters for the silver or copper atoms. As an example of the application of this method, we have reinvestigated the crystal structure of samsonite, $Ag_4MnSb_2S_6$.

Keywords: Crystal structure, samsonite, X-ray data, atomic displacement parameters